## (Q)SAR reporting template CAR Document IIIA

In case you don’t use IUCLID for reporting the (Q)SAR estimation, complete the template below, which is based on the harmonised IUCLID template. Applicants should provide the filled template as a Doc IIIA document to the CAR. Please refer for further instructions and examples to QSAR Practical Guide sections 3.4 *How to report a (Q)SAR prediction in IUCLID* & 4. *Practical examples*.

### Administrative data

**Endpoint**

**Adequacy of study**

|  |  |
| --- | --- |
|  | key study |
|  | supporting study |
|  | weight of evidence |
|  | disregarded due to major methodological deficiencies |
|  | other information |

**Reliability**

|  |  |
| --- | --- |
|  | 1 (reliable without restriction) |
|  | 2 (reliable with restrictions) |
|  | 3 (not reliable) |
|  | 4 (not assignable) |
|  | other |

**Rationale for reliability incl. deficiencies**

|  |  |
| --- | --- |
|  | results derived from a valid (Q)SAR model and falling into its applicability domain, with adequate and reliable documentation / justification (Reliability 1 or 2) |
|  | results derived from a valid (Q)SAR model and falling into its applicability domain, With limited documentation / justification (Reliability 2, 3 or 4) |
|  | results derived from a valid (Q)SAR model, but not (completely) falling into its applicability domain, With adequate and reliable documentation / justification (Reliability 2 or 3) |
|  | results derived from a (Q)SAR model, with limited documentation / justification, but validity of model and reliability of prediction considered adequate based on a generally acknowledged source (reliability 2 or 3) |
|  | results derived from a valid (Q)SAR model, but not (completely) falling into its applicably domain, and documentation / justification is limited (Reliability 3 or 4) |
|  | results derived from a (Q)SAR model, with limited documentation / justification (Reliability 4) |
|  | other: |

**Justification for type of information**

Either populate the fields below or attach files for QMRF (validity of the model) and QRPF (applicability of the model to a specific substance).

1 Software w

2 Model (incl. version number)

3 Smiles or other identifiers as input for the model

4 Scientific validity of the (Q)SAR model

(Explain how the model fulfils the OECD principles for (Q)SAR model validation. Consider attaching the QMRF or Providing a link)

- Defined endpoint:

- Unambiguous algorithm

- Defined domain of applicability

- Appropriate measures of goodness-of-fit and robustness and predictivity

- Mechanistic interpretation

5 Applicability domain

(Explain how the substance falls within the applicability domain of the model)

- Descriptor domain

- Structural and mechanistic domains:

- Similarity With analogues in the training set

- Other considerations (as appropriate)

6 Adequacy of the result

(Explain how the prediction fits the purpose of classification and labelling and/or risk assessment)

### Data source

**Reference**

Title

Author

Reference type

Year

Bibliographic source

**Data access**

|  |  |
| --- | --- |
|  | data submitter is data owner |
|  | data submitter has Letter of Access |
|  | data no longer protected |
|  | data published |
|  | not applicable |
|  | data submitter has permission to refer |
|  | other |

**Data protection claimed**

|  |  |
| --- | --- |
|  | yes |
|  | yes, but willing to share  |
|  | yes, but not willing to share |

### Materials and methods

**Principles of method**

### Test materials

**Test material information**

**Specific details on test material used for the study**

### Results and discussion

**(Q)SAR predicted results**

**Any other information on results including tables**